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Introduction

As part of the Idaho National Laboratory's (INL's) Secure Energy Initiative, the INL is performing research in areas that are vital to ensuring clean, secure energy supplies for the future. The INL Hybrid Energy Systems Testing (HYTEST) Laboratory is being established to develop and test hybrid energy systems with the principal objective to safeguard U.S. Energy Security by reducing dependence on foreign petroleum. HYTEST involves producing liquid fuels in a Hybrid Energy System (HES) by integrating carbon-based (i.e., bio-mass, oil-shale, etc.) with non-carbon based energy sources (i.e., wind energy, hydro, geothermal, nuclear, etc.). Advances in process development, control and modeling are the unifying vision for HES.

This paper describes new modeling tools and methodologies to simulate advanced energy processes. Needs are emerging that require advanced computational modeling of multiphase reacting systems in the energy arena, driven by the 2007 Energy Independence and Security Act, which requires production of 36 billion gal/yr of biofuels by 2022, with 21 billion gal of this as advanced biofuels. Advanced biofuels derived from microalgal biomass have the potential to help achieve the 21 billion gal mandate, as well as reduce greenhouse gas emissions. Production of biofuels from microalgae is receiving considerable interest due to their potentially high oil yields (around 600 gal/acre). Microalgae have a high lipid content (up to 50%) and grow 10 to 100 times faster than terrestrial plants. Figure 1 shows the experimental facilities for studying algal biofuel production at the Idaho National Laboratory.

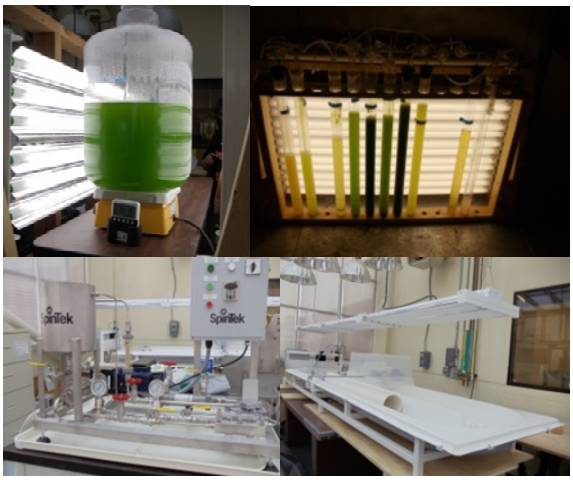

Figure 1. Algal biofuel laboratory at the Idaho National Laboratory.

The use of environmentally friendly alternatives to solvents and reagents commonly employed in reaction and phase separation processes is being explored. This is accomplished through the use of hydrothermal technologies, which are chemical and physical transformations in high-temperature (200–600 °C), high-pressure (5–40 MPa) liquid or supercritical water. Figure 2 shows a simplified diagram of the production of biofuels from algae. Hydrothermal processing has significant advantages over other biomass processing methods with respect to separations. These "green" alternatives employ a hybrid medium that, when operated supercritically, offers the prospect of tunable physicochemical properties. Solubility can be rapidly altered and phases partitioned selectively to precipitate or dissolve certain components by altering temperature or pressure in the near-critical region.[1] The ability to tune the solvation properties of water in the highly compressible near-critical region facilitates partitioning of products or by-products into separate phases to separate and purify products. Since most challenges related to lipid extraction are associated with the industrial scale-up of integrated extraction systems, the new modeling capability offers the prospect of addressing previously untenable scaling issues.

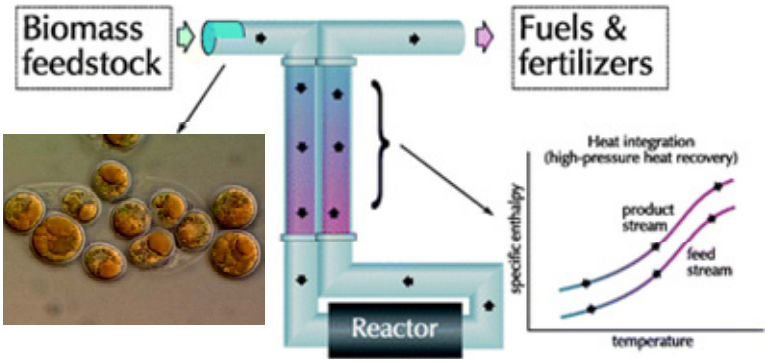

Figure 2. Conceptual diagram illustrating the production of biofuels in hydrothermal media.[1]

The objective of this research is to develop and validate a new computational multiphase fluid dynamics (CMFD) tool to model lipid extraction from microalgae using biphasic mixtures of supercritical carbon dioxide and water. Modeling can provide essential information on feasibility, optimization and scale-up of the proposed algal-to-biofuels process. Over the next three years, we will be developing the MultiphasE Eulerian Reactive Chemistry and Transport (MEERCAT) code built upon the Multiphysics Object Oriented Simulation Environment (MOOSE) library developed at INL to facilitate solution of computationally intensive problems via massive parallelism. MOOSE has been evolving rapidly due to the requirements of a host of applications that are being built upon it. The MEERCAT code is based upon a modern programming paradigm and will have the following features:

- Built on INL's Multiphysics MOOSE library, which provides a strong numerical foundation for rapid development of multidimensional, parallel, implicit, fully coupled, nonlinear simulation capabilities
- Flexible, modular systems for defining physics, material properties, chemical reactions, boundary conditions and custom submodels
- Scaleable parallelism to achieve practical simulation times for computationally stiff problems (i.e., those incorporating disparate time scales)
- Adaptive mesh refinement/coarsening for improved resolution and reduced meshing/computing time

Methodology

MEERCAT is being developed with state-of-the-art modeling tools to provide the capability to assess and visualize fluid flow, chemical reactions, mass transport phenomena, and heat transfer. This robust, parallel scalable modeling capability is based on MOOSE [2]. MOOSE incorporates the benefits of object-oriented design (OOD), wherein objects with defined interfaces are manipulated. Implementation details are hidden from the user using elements of OOD, such as data encapsulation, inheritance and polymorphism. MOOSE supports rapid development of engineering-scale simulations by leveraging existing discretization and solver technologies [3-5] and organizing multiphysics calculations into a collection of interacting single physics components called *Kernels*. Kernels provide a modular approach to incrementally developing complex multiphysics simulations. Kernels are discrete physics modules that can easily be added, swapped or coupled together. Figure 3 illustrates the MOOSE framework. MOOSE has been effectively used to develop multiphysics applications in nuclear fuel performance [6], high-temperature gas-cooled pebble bed reactors [7], phase-field simulation of microstructural evolution of materials [8], and enhanced geothermal systems [9]. Recent experience in developing these applications indicates that MOOSE can reduce the cost of developing complex multiphysics applications from tens of man-years to less than one man-year.

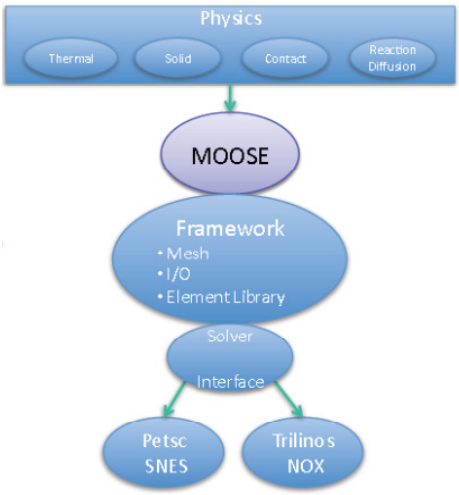

Figure 3. Schematic of MOOSE framework.

As a first step in the development of the code, governing equations for multiphase phase reacting flow with transport of heat are defined. The basic architecture of the code allows for convenient coupling of different processes and incorporation of new physics. We will begin the effort with an initial implementation of multiphase flow: conservation of mass, momentum and energy for each of the phases and a model for mass transfer between the phases. In the Eulerian-Eulerian (EE) formulation, the different fluid phases are treated as interpenetrating continua. The EE approach offers the computational advantage of identical parallelization of liquid and gas solvers [10]. The probability of each phase at any location is indicated by the volume fraction.

MOOSE utilizes a Galerkin finite element based solution method. Finite element methods (FEM) are a subset of the method of weighted residuals wherein a particular function space is chosen to represent the function to solve for and the function to weight against. In this method, a weighted residual equation is formed:

$$R_i = \iiint W_i Q dV^e$$

where R_i is the equation residual at an element vertex i, Q is the conservation equation expressed on an element basis, W_i is the weight factor and V^e is the volume of the element. The input that must be supplied for this method is known as the "weak form" of partial differential equations. Weak forms are generated by multiplying a partial differential equation by a weighting function and then integrating over the domain. The FEM formulation requires special care to ensure a conservative solution. Generally stability/robustness of the solution is better in FEM, even though it might require more memory than finite-volume methods [11]. For these reasons, FEM is a new direction in which CFD is moving.

In general, because of the high reaction rate, species conservation equations become very stiff; traditionally, small time steps are used to overcome this stiffness problem. However, such an approach places severe restrictions on the time-step because the flow time scales associated with certain domains, such as recirculation and co-flow entrainment regions are several orders of magnitude larger than the chemical time scales. However, the implicit solution procedures used by MOOSE permit stable calculations without untenably small time-steps. Numerical experiments may be performed by increasing the reaction rates in an attempt to approach asymptotically infinitely thin reaction zones. Increasing the reaction rates renders the species conservation equations stiffer and challenges the numerical algorithm in handling stiff equations.

MOOSE supports Jacobian-free Newton-Krylov (JFNK) methods for solution of tightly coupled multiphysics problems [12]. The robustness and efficiency of JFNK is determined by the preconditioner that is used to approximately solve the linearized system at each Newton step. A number of approaches to preconditioning are possible, not least of which is adapting existing operator-split solution techniques as preconditioners; see, for example [13], where the SIMPLE and SIMPLER algorithms are adapted for this purpose in the context of

incompressible flow. Facilitated by MOOSE's flexibility and leveraging of existing state-of-the-art solver technology [4, 5], our initial focus will be on finding an effective preconditioning strategy that scales favorably with mesh resolution and is robust with respect to flow parameters. Following this we will add chemical reactions. A particular challenge will be proper handling of the turbulence model. Different approaches based on directly including turbulence equations in the multiphase model or solving them in a more loosely coupled (yet consistent) fashion will be explored.

Through its leverage of external simulation capabilities, MOOSE offers advanced simulation tools that we will deploy in this project. In particular, MOOSE can take advantage of libMesh services for adaptive mesh refinement. The accuracy of a simulation performed using an LES scheme depends on the grid resolution. Spatial discretization using *unstructured grids* will be implemented in order to allow for arbitrary geometries and adaptive refinement. libMesh provides tools for identifying locations where greater resolution is needed and handles the required regridding operations, such as mesh generation and transfer of information between grids. An important outcome of this effort will be determining the suitability of dynamic adaptive mesh refinement in regions characterized by complex dynamics. In addition, new libMesh capabilities for adjoint-based error estimation and sensitivity analysis are currently under development. The latter will be of particular use to investigate the sensitivity of model output to model parameters such as mass transfer coefficients and reaction kinetic terms during calibration and validation efforts. Leveraging what has been done in MOOSE will allow us to solve complex problems without having to create a framework from scratch for a multiphase, reacting flow code.

The attractive features of MOOSE include plug-and-play modules to enable simplified coupling. MOOSE provides a set of interfaces and framework to access a core set of common services (i.e., libMesh: http://libmesh.sf.net). The solver interface abstracts specific solver implementations with a common interface to modern linear and nonlinear solvers. These robust solvers are key for ease of use and modularity.

High-performance computing can significantly reduce the time required for complex calculations, often from months to days, and offers the memory capacity required for high resolution of complex multicomponent phenomena. Computations will be executed on INL's *fission* cluster, a 12,512 core Appro distributed memory system with 391 compute nodes with four (4) processor sockets per node. The system features 2.4GHz AMD Magny-Cours 8-core processors with 2 GB memory/core and 25TB total memory. The LINPACK benchmark for this system is 90+ Tflops.

Description of Virtual Laboratory Environment

The ultimate vision for this work is to create a "Virtual Laboratory" environment, where the user interacts with a multi-modal, tele-immersive virtual reality environment. Currently available massively parallel supercomputers provide sufficient performance to simulate multi-dimensional, multi-variable problems in high resolution. Related efforts in sensitivity analysis, parallelization, and scientific visualization are being undertaken. We plan to utilize advanced scientific visualization techniques to examine the results of the simulations in order to improve our understanding of the complex interactions among flow transport processes and chemical reactions. Scientific visualization focuses on the use of computer graphics to create visual images which aid in understanding of complex, often massive numerical representation of scientific concepts or results [14]. It conveys insight by leveraging the bandwidth of human visual perception to help identify patterns and relationships contained in data. Graphical representations of numerical data for their qualitative and quantitative analysis will aid in developing and validating our model, as well as communicating our results to a broader audience. Interactive visualization capabilities enable the analysis and assessment of large modeling and simulation data sets. Especially for complex models, visualization is key to understanding interacting physico-chemical processes occurring in the system.

However, visualization of large amounts of result data is cumbersome with traditional methods, where postprocessing modules are usually coupled to the raw data source - either by files or by data flow. In this paper we describe an efficient, distributed system approach to support three-dimensional, interactive exploration of complex results of scientific computing. Virtual objects are displayed in INL's Computer Aided Visualization Environment (CAVE) by taking advantage of high-quality rendering, stereoscopic displays and interactive navigation and tracking devices.

Interactive visualization capabilities enable the analysis and assessment of complex modeling and simulation results. A PowerWall consisting of a rear projector-based system provides a 6 × 12-ft display using six DLP™ projectors in a 3 × 2 matrix configuration, each providing 1,400 × 1,050 resolution that results in a 7.1 mega-pixel display. It is driven by a small visualization cluster consisting of three nodes each comprised of a pair of dual-core microprocessors for a total of 12 computing cores, with each node providing 16 GB memory. The projection system seamlessly blends the images from each projector and automatically balances color and light to produce a bright, high quality display. A second, smaller PowerWall is also available. A display wall integrating the instrumentation and controls, process models, experimental data and simulations is planned for operation at the HYTEST facility.

A code agnostic visualization interface will be employed suitable for use with other codes built on the `MOOSE` platform. These analysis tools will provide the domain research scientists with methods of exploring their data that currently do not exist or are overly difficult to use. Emphasis will be placed on devising an intuitive user interface that will serve as a conduit to discovery rather than the bottleneck between the data and the scientist. We will also explore immersive interfaces that allow the user to both observe and interact with the full three dimensional volume of data. The unique contributions of the visualization effort will include multidimensional transfer functions to distinguish different constituents, species, and features in the flow; track their evolution through future time steps; and a natural user interface that takes advantage of inherent three-dimensional human capabilities. An initial set of tools might include a three-dimensional linear and volumetric measurement tool; a multi dimensional transfer function for separating different constituents; and a feature tracking tool to follow individual phases. We will also seek to develop approaches to visualize the results of parameter sensitivities. We expect that the interplay between visualization and sensitivity analysis will facilitate scientific discovery.

Verification and Validation (V&V)

Verification and validation (V&V) will be done in accordance with the ASME V&V 20 Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer [15]. The simulation will be guided by a validation hierarchy. Techniques, such as the Method of Manufactured Solutions [16-18], are used to verify that the set of equations are being solved correctly. The validation hierarchy will employ a systematic approach that will ultimately lead to a model with the ability to accurately solve multiphase flow problems. This approach builds upon validation at the lower levels. Detailed flow field comparisons with experimental data will be done to assess the code's ability to accurately model the underlying physics of the flow, from the physics to the submodels to the bench-scale to the pilot-scale and ultimately to the production scale. Experimental results will support reactor modeling and model validation. In turn, the modeling effort will assist in the design of experiments.
The product resulting from this project will be a fully functional and validated model of multiphase, reacting flow. `MEERCAT` will be designed with capabilities for sensitivity analysis that can be used to improve the fidelity of the model and to help focus the design of experiments.

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